```
data_lach25

_publ_section_comment
;
Solvent is present in the structure, a water molecule is above the
cobalt ion and a disordered
DMF molecule is above this. The positions of these molecules are
disorder and the exact positions
are not determined.
;

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_chemical_formula_weight          3554.47

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 'H'  'H'   0.0000   0.0000
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 'O'  'O'   0.0492   0.0322
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Si'  'Si'   0.2541   0.3302
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'P'  'P'   0.2955   0.4335
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 'W'  'W'  -5.4734   5.5774
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Co'  'Co'  -2.3653   3.6143
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0311   0.0180
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'R 3 m'

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 '-y, x-y, z'
 '-x+y, -x, z'
 '-x+y, y, z'
 'x, x-y, z'
 '-y, -x, z'
 'x+2/3, y+1/3, z+1/3'
 '-y+2/3, x-y+1/3, z+1/3'
 '-x+y+2/3, -x+1/3, z+1/3'
 '-x+y+2/3, y+1/3, z+1/3'
 'x+2/3, x-y+1/3, z+1/3'
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 'x+1/3, y+2/3, z+2/3'
 '-y+1/3, x-y+2/3, z+2/3'
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 '-x+y+1/3, y+2/3, z+2/3'
 'x+1/3, x-y+2/3, z+2/3'
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_cell_angle_gamma                 120.00
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_cell_formula_units_Z             3
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_computing_data_reduction         SAINTPLUS
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_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
wR and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
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^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_abs_structure_details
 'Flack H D (1983), Acta Cryst. A39, 876-881'
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_refine_ls_wR_factor_ref          0.1040
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_refine_ls_goodness_of_fit_ref    1.041
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C1 C 0.4540(6) 0.5460(6) 0.0212(9) 0.067(4) Uani 1 2 d SU . .
C2 C 0.4458(8) 0.5542(8) 0.0855(9) 0.102(8) Uani 1 2 d SU . .
H2 H 0.4220 0.5780 0.0996 0.122 Uiso 1 2 calc SR . .
```

C3 C 0.4744(9) 0.5256(9) 0.1274(11) 0.122(8) Uani 1 2 d SU . .
H3 H 0.4695 0.5305 0.1704 0.146 Uiso 1 2 calc SR . .
C4 C 0.5098(8) 0.4902(8) 0.1081(12) 0.113(7) Uani 1 2 d SU . .
C5 C 0.5160(8) 0.4840(8) 0.0466(13) 0.137(12) Uani 1 2 d SU . .
H5 H 0.5396 0.4604 0.0320 0.165 Uiso 1 2 calc SR . .
C6 C 0.4875(7) 0.5125(7) 0.0032(12) 0.112(10) Uani 1 2 d SU . .
H6 H 0.4926 0.5074 -0.0397 0.135 Uiso 1 2 calc SR . .
C7 C 0.5372(11) 0.4628(11) 0.1577(17) 0.154(11) Uani 1 2 d SU . .
H7 H 0.5298 0.4702 0.1996 0.185 Uiso 1 2 calc SR . .
C8 C 0.5694(13) 0.4306(13) 0.145(3) 0.26(2) Uani 1 2 d SU . .
H8A H 0.5770 0.4230 0.1037 0.312 Uiso 1 2 calc SR . .
H8B H 0.5862 0.4138 0.1779 0.312 Uiso 1 2 calc SR . .
C9 C 0.4140(13) 0.4704(14) 0.6638(13) 0.160(9) Uani 1 1 d DU . .
H9A H 0.4150 0.4696 0.7094 0.192 Uiso 1 1 calc R . .
H9B H 0.3923 0.4989 0.6513 0.192 Uiso 1 1 calc R . .
C10 C 0.3665(15) 0.3923(14) 0.6393(15) 0.182(13) Uani 1 1 d DU . .
H10A H 0.3694 0.3930 0.5936 0.219 Uiso 1 1 calc R . .
H10B H 0.3866 0.3634 0.6546 0.219 Uiso 1 1 calc R . .
C11 C 0.2920(16) 0.3573(16) 0.6567(16) 0.171(10) Uani 1 1 d DU . .
H11A H 0.2719 0.3860 0.6410 0.206 Uiso 1 1 calc R . .
H11B H 0.2893 0.3572 0.7024 0.206 Uiso 1 1 calc R . .
C12 C 0.2465(18) 0.284(2) 0.635(2) 0.251(19) Uani 1 1 d DU . .
H12A H 0.1977 0.2665 0.6480 0.376 Uiso 1 1 calc R . .
H12B H 0.2633 0.2534 0.6526 0.376 Uiso 1 1 calc R . .
H12C H 0.2486 0.2824 0.5898 0.376 Uiso 1 1 calc R . .
C13 C 0.4938(7) 0.5062(7) 0.5692(15) 0.143(9) Uani 1 2 d SU . .
H13A H 0.5439 0.5289 0.5562 0.171 Uiso 0.50 1 calc PR . .
H13B H 0.4711 0.4561 0.5562 0.171 Uiso 0.50 1 calc PR . .
C14 C 0.4602(9) 0.5398(9) 0.5332(18) 0.188(11) Uani 1 2 d SDU . .
H14A H 0.4829 0.5908 0.5430 0.226 Uiso 0.50 1 calc PR . .
H14B H 0.4092 0.5171 0.5430 0.226 Uiso 0.50 1 calc PR . .
C15 C 0.4718(15) 0.5282(15) 0.459(2) 0.230(16) Uani 1 2 d SDU . .
H15A H 0.5227 0.5511 0.4491 0.276 Uiso 0.50 1 calc PR . .
H15B H 0.4489 0.4773 0.4491 0.276 Uiso 0.50 1 calc PR . .
C16 C 0.4353(19) 0.5647(19) 0.425(3) 0.34(3) Uani 1 2 d SDU . .
H16A H 0.4410 0.5621 0.3800 0.517 Uiso 1 2 calc SR . .
H16B H 0.4574 0.6143 0.4374 0.517 Uiso 0.50 1 calc PR . .
H16C H 0.3849 0.5403 0.4350 0.517 Uiso 0.50 1 calc PR . .
C17 C 0.5285(8) 0.4715(8) 0.6651(13) 0.134(9) Uani 1 2 d SDU . .
H17A H 0.5777 0.4953 0.6497 0.160 Uiso 0.50 1 calc PR . .
H17B H 0.5047 0.4223 0.6497 0.160 Uiso 0.50 1 calc PR . .
C18 C 0.5304(11) 0.4696(11) 0.7356(16) 0.21(2) Uani 1 2 d SDU . .
H18A H 0.5543 0.5188 0.7511 0.255 Uiso 0.50 1 calc PR . .
H18B H 0.4812 0.4457 0.7511 0.255 Uiso 0.50 1 calc PR . .
C19 C 0.5664(11) 0.4336(11) 0.7622(18) 0.25(2) Uani 1 2 d SDU . .
H19A H 0.6166 0.4572 0.7492 0.301 Uiso 0.50 1 calc PR . .
H19B H 0.5428 0.3834 0.7492 0.301 Uiso 0.50 1 calc PR . .
C20 C 0.5601(13) 0.4399(13) 0.835(2) 0.27(3) Uani 1 2 d SDU . .
H20A H 0.5850 0.4191 0.8563 0.406 Uiso 1 2 calc SR . .
H20B H 0.5102 0.4146 0.8470 0.406 Uiso 0.50 1 calc PR . .
H20C H 0.5813 0.4898 0.8465 0.406 Uiso 0.50 1 calc PR . .
O1 O 0.5081(5) 0.7540(3) -0.1466(5) 0.046(2) Uani 1 2 d SU . .
O2 O 0.5776(4) 0.6781(5) -0.1750(5) 0.070(2) Uani 1 1 d U . .
O1S O 0.3333 0.6667 0.1424(7) 0.022(3) Uiso 1 6 d SU . .
O3 O 0.4816(4) 0.6362(5) -0.0762(5) 0.0560(18) Uani 1 1 d U . .
O4 O 0.4414(3) 0.5586(3) -0.1830(6) 0.050(2) Uani 1 2 d SU . .
O5 O 0.3751(2) 0.6249(2) -0.1523(5) 0.0330(19) Uani 1 2 d SU . .
O6 O 0.4729(4) 0.6769(4) -0.2519(4) 0.0434(16) Uani 1 1 d U . .
O7 O 0.3754(3) 0.6246(3) -0.3454(5) 0.053(3) Uani 1 2 d SU . .
O8 O 0.3333 0.6667 -0.2506(7) 0.032(3) Uani 1 6 d SU . .
O9 O 0.5025(7) 0.7512(4) -0.3667(6) 0.073(3) Uani 1 2 d SU . .
O10 O 0.3830(3) 0.6170(3) -0.0061(9) 0.081(4) Uani 1 2 d SU . .
Si1 Si 0.3333 0.6667 -0.1725(4) 0.0254(12) Uani 1 6 d SU . .
P1 P 0.41688(13) 0.58312(13) -0.0349(4) 0.0604(11) Uani 1 2 d SU . .
W1 W 0.49130(3) 0.66063(3) -0.1680(3) 0.04549(17) Uani 1 1 d U . .
W2 W 0.43711(4) 0.71855(2) -0.3111(3) 0.0465(2) Uani 1 2 d SU . .

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Co1 Co 0.3333 0.6667 0.0310(4) 0.0636(13) Uani 1 6 d SU . .
N1 N 0.4928(6) 0.5072(6) 0.6384(12) 0.141(4) Uani 1 2 d SU . .
C1S C 0.3333 0.6667 0.4687 0.45(10) Uiso 1 6 d SDU . .
H1S H 0.3079 0.6826 0.4930 0.540 Uiso 0.17 1 calc PR . .
O2S O 0.3731 0.6269 0.4901 0.53(17) Uiso 0.33 2 d SPDU . .
N1S N 0.3468 0.6734 0.3955 0.42(8) Uiso 0.33 2 d SPDU . .
C3S C 0.3461 0.6173 0.3324 0.35(8) Uiso 0.33 1 d PDU . .
H3S1 H 0.3908 0.6420 0.3097 0.528 Uiso 0.33 1 calc PR . .
H3S2 H 0.3068 0.6067 0.3044 0.528 Uiso 0.33 1 calc PR . .
H3S3 H 0.3403 0.5731 0.3494 0.528 Uiso 0.33 1 calc PR . .

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C2 0.134(17) 0.134(17) 0.060(7) 0.011(4) -0.011(4) 0.084(17)
C3 0.172(17) 0.172(17) 0.052(10) 0.017(5) -0.017(5) 0.109(18)
C4 0.136(14) 0.136(14) 0.083(10) 0.027(5) -0.027(5) 0.081(15)
C5 0.20(3) 0.20(3) 0.095(11) 0.017(5) -0.017(5) 0.16(3)
C6 0.16(2) 0.16(2) 0.076(10) 0.014(4) -0.014(4) 0.13(2)
C7 0.173(18) 0.173(18) 0.131(17) 0.046(9) -0.046(9) 0.097(19)
C8 0.32(4) 0.32(4) 0.25(4) 0.062(12) -0.062(12) 0.26(4)
C9 0.155(11) 0.163(16) 0.20(2) -0.049(16) 0.051(14) 0.110(9)
C10 0.175(15) 0.155(17) 0.24(3) -0.05(2) 0.05(2) 0.100(9)
C11 0.172(15) 0.157(19) 0.21(3) -0.02(2) 0.04(2) 0.102(11)
C12 0.18(2) 0.19(3) 0.38(6) -0.07(3) -0.04(3) 0.091(14)
C13 0.18(2) 0.18(2) 0.151(8) -0.035(4) 0.035(4) 0.15(2)
C14 0.22(2) 0.22(2) 0.219(15) -0.015(7) 0.015(7) 0.17(2)
C15 0.26(3) 0.26(3) 0.187(14) 0.008(10) -0.008(10) 0.15(3)
C16 0.39(4) 0.39(4) 0.31(3) 0.06(2) -0.06(2) 0.24(4)
C17 0.15(2) 0.15(2) 0.138(12) -0.032(5) 0.032(5) 0.10(2)
C18 0.28(5) 0.28(5) 0.138(14) -0.034(7) 0.034(7) 0.19(5)
C19 0.32(5) 0.32(5) 0.17(2) 0.004(10) -0.004(10) 0.20(6)
C20 0.39(7) 0.39(7) 0.18(2) -0.014(10) 0.014(10) 0.30(7)
O1 0.034(5) 0.051(4) 0.048(5) -0.003(2) -0.007(4) 0.017(3)
O2 0.050(4) 0.081(6) 0.086(6) 0.000(5) -0.001(4) 0.039(5)
O3 0.052(4) 0.060(5) 0.061(4) 0.003(3) -0.015(3) 0.031(4)
O4 0.055(4) 0.055(4) 0.055(6) -0.002(2) 0.002(2) 0.039(5)
O5 0.029(3) 0.029(3) 0.040(5) 0.0010(18) -0.0010(18) 0.013(4)
O6 0.035(4) 0.047(4) 0.053(4) -0.002(3) 0.010(3) 0.024(4)
O7 0.065(4) 0.065(4) 0.037(5) -0.007(2) 0.007(2) 0.038(5)
O8 0.034(5) 0.034(5) 0.027(6) 0.000 0.000 0.017(2)
O9 0.073(7) 0.089(7) 0.053(6) 0.009(3) 0.017(5) 0.037(4)
O10 0.071(7) 0.071(7) 0.114(12) 0.006(3) -0.006(3) 0.046(8)
Si1 0.0274(18) 0.0274(18) 0.021(3) 0.000 0.000 0.0137(9)
P1 0.067(2) 0.067(2) 0.052(2) 0.0046(10) -0.0046(10) 0.037(2)
W1 0.0365(3) 0.0522(4) 0.0532(3) 0.0019(2) -0.0003(2) 0.0262(3)
W2 0.0465(5) 0.0529(4) 0.0379(4) 0.00575(16) 0.0115(3) 0.0232(2)
Co1 0.074(2) 0.074(2) 0.043(2) 0.000 0.000 0.0370(11)
N1 0.158(6) 0.158(6) 0.157(7) -0.043(3) 0.043(3) 0.117(7)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
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 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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C1 P1 1.821(18) . ?
C2 C3 1.38(3) . ?
C3 C4 1.38(4) . ?
C4 C5 1.32(4) . ?
C4 C7 1.46(4) . ?
C5 C6 1.40(3) . ?
C7 C8 1.22(6) . ?
C9 C10 1.55(3) . ?
C9 N1 1.56(2) . ?
C10 C11 1.43(3) . ?
C11 C12 1.45(3) . ?
C13 C14 1.46(5) . ?
C13 N1 1.47(3) . ?
C14 C15 1.62(4) . ?
C15 C16 1.54(4) . ?
C17 N1 1.44(3) . ?
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C18 C19 1.45(4) . ?
C19 C20 1.56(4) . ?
O1 W1 1.901(3) 5_565 ?
O1 W1 1.901(3) . ?
O2 W1 1.698(8) . ?
O1S Co1 2.362(13) . ?
O3 P1 1.551(9) . ?
O3 W1 2.000(8) . ?
O4 W1 1.918(5) . ?
O4 W1 1.918(5) 6_665 ?
O5 Si1 1.607(9) . ?
O5 W1 2.231(6) 6_665 ?
O5 W1 2.231(6) . ?
O6 W1 1.892(8) . ?
O6 W2 1.909(8) . ?
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O8 Si1 1.657(16) . ?
O8 W2 2.313(8) 2_665 ?
O8 W2 2.313(8) 3_565 ?
O8 W2 2.313(8) . ?
O9 W2 1.691(12) . ?
O10 P1 1.396(15) . ?
O10 Co1 2.003(14) . ?
Si1 O5 1.607(9) 2_665 ?
Si1 O5 1.607(9) 3_565 ?
P1 O3 1.551(9) 6_665 ?
W2 O6 1.909(8) 5_565 ?
W2 O7 1.913(5) 2_665 ?
Co1 O10 2.003(14) 2_665 ?
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C1S N1S 1.5736(7) . ?
N1S N1S 0.4319 3_565 ?
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N1S C3S 1.7933(5) 5_565 ?

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